Planetary Data Systems Internship - Final Report

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Abstract

In this report, I outline the progress made and challenges faced in my time as a student investigator on the Planetary Data Systems internship program.

Research Question

The central research question of my project was defined as follows:

How do fluctuations in surface relative humidity affect tropical surface temperatures on Earth-like planets?

Relative humidity represents water vapour in the atmosphere, among the strongest greenhouse gases known to man. It has historically been presumed to be static and unchanging, a trend apparent in modern climate models. Recent evidence points instead to gradual changes over long periods of time. What has been/could be the impact of this hitherto unaccounted change on the climate of our planet and other planets?

This project was conceived and executed independently by myself as an undergraduate at the University of California, Los Angeles, with funding received from the NASA Planetary Data Systems division.

Background

Project Description

As a member of the 2013-2015 NASA Planetary Data Systems cohort, I worked with Prof. Aradhna Tripati at UCLA to investigate the impact of long-term (> 10 years) changes in relative humidity on tropical sea surface temperatures. The project had two aspects: a modeling component, where we would attempt to simulate the effects on temperatures in a one-dimensional radiative atmosphere numerically, using modern sea surface temperature data and relative humidity change rates found in Katharine M. Willett's doctoral thesis[1]; and an experimental component, where we would attempt to reconstruct temperatures from the last 25,000 years using clumped isotope thermometry on lake snail shells obtained from Lake Tuwoti, Indonesia, and compare the results to the predictions of our model.

The idea was to be able to obtain a first approximation to the effect of changes in long-term relative humidity for both past and present. As a side benefit, this study would also constrain existing temperatures in the Tropics between the period of the last glacial maximum (conventionally abbreviated to the LGM, ca. 20,000 years before present) and modern times - something for which there is currently little data available. It fits in with the NASA Planetary Data Systems (PDS) internship by constraining the influence of water vapor in the evolution of planetary tropical climates, allowing us to discern whether planets that appear capable of supporting life are indeed capable of doing so.

[1] *Creation and Analysis of HadCRUH: a New Global Surface Humidity Dataset*, Katharine M. Willett, March 2007, `http://www.cru.uea.ac.uk/cru/pubs/thesis/2007-willett/`

Methodology

This section elaborates on the methods we used to carry out the work described above, highlighting the connection with NASA PDS products.

Data for the modeling component came from three sources: spectrometric data for water vapour from the 1990 mission Geologic Remote Sensing Field Experiment (GRSFE), currently hosted on the Geosciences node of the PDS website; remote sensing data about relative humidity throughout the atmosphere from the MODIS (moderate resolution imaging spectrometer) and AIRS (atmospheric infrared spectrometer) instruments aboard NASA's Aqua satellite, obtained from Goddard Earth Sciences Data and Information Services Center (GES DISC); and relative humidity trends between 1970-1990 from Katherine Willett's PhD thesis (see footnote reference).

Data for the experimental component consisted of calibrated inferences of temperature from concentrations of rare molecules - known otherwise as clumped isotope thermometry - in snail shell samples obtained from carefully preserved samples from Lake Tuwoti, Indonesia. Our choice of clumped isotope thermometry was motivated by the fact that other paleoclimatic reconstruction methods (such as $\delta^{18}O$ paleothermometry) are not based purely on thermodynamic effects and thus tend to be prone to non-thermodynamic biases such as fluid composition, preferential Mg/Ca enrichment, etc.

The model, as originally conceived, focused on three fundamental aspects of a one-dimensional atmosphere:

- Cloud distribution and cover
- Water vapour distribution at various heights, parameterised by water vapour pressure
- Greenhouse models and temperature lapse-rates

The atmosphere itself was modelled as a series of layers with a strict temperature lapse rate between them. Heat would come in from solar radiation, diffuse itself across layers which would warm up slightly due to the specific heat of water vapour, and re-radiate in all directions as an approximate blackbody. Cloud formation would occur once the temperature-dependent saturation water vapour pressure was reached in a layer, leading to much larger reflection of all heat. Once layer temperatures came to be stable, the relative humidity would be slowly altered, and the resulting behaviour of the toy system recorded. Details about the model - including relevant equations with empirical backing - were sourced from extensive literature review, and can be found in my initial proposal for the PDS program.

Clumped isotope thermometry makes use of rare isotopologues of carbon dioxide molecules that are preferentially formed at colder temperatures. By measuring the ratio of these isotopologues to 'ordinary' carbon dioxide with a mass spectrometer, one can determine the temperature of formation of an organic substance using a calibration scale. Samples undergo conversion to gaseous CO_2 form on reaction with orthophosphoric acid, with a distillation system cleaning out non-carbon dioxide elements before being fed into a customised Thermofisher MAT 23 spectrometer.

Progress

Progress was made on the experimental front:

- Following literature review and training, the period of January - March 2014 was devoted to the pre-processing, cleaning and eventual analysis of our samples. Samples were washed, sonicated, freeze-dried, treated with hydrogen peroxide to remove organic contamination, and partially crushed into powder for mass spectrometric analysis. Owing to the low estimated carbon-containing content ($< 1\,\%$) of the samples in reports of the sample excavation team, sample powder was prepared in bulk quantities exceeding usual analytic limits (150 mg versus usual 10 - 12 mg) on expert recommendation.

Progress was made on the theoretical front:

- Following literature review and data download from NASA GES DISC and PDS systems, a model was constructed in Python between June to August 2014. Data was pre-processed during this stage. Parameters for miscellaneous elements in the model - e.g. layer size and number, atmospheric constituent levels, layer transmissivity, etc. - were taken from McKay and Khalil[2]. Eighteen layers of the atmosphere were

[2] *Theory and Development of a One-Dimensional Time Dependent Radiative Convective Model*, R.M. MacKay, M.A. Khalil, Chemosphere. Vol. 22, Nos 3-4, pp. 383-417, 1991

simulated, with prescribed oxygen and nitrogen dioxide concentrations, in accordance with McKay and Khalil's procedure. Atmospheric temperature was used as the primary independent variable governing values for specific heat, dewpoint, and saturation water vapour pressure.

- It was discovered that reconstructing relative humidities in the past, assuming a closed lake system with little to no runoff, is possible via a combination of analysis of the $\delta^{18}O$ content (roughly, the proportion of stable ^{18}O isotopes in the system) using the principles outlined in Wolfe et al.[3] and clumped isotope thermometry. In particular, Wolfe relied on the phenomenon that rainfall is ^{16}O enriched, since evaporation preferentially favours lighter isotopes, meaning that lake systems tend to have larger ^{18}O levels - since evaporation rates are constrained by relative humidity, one can use ^{18}O records to estimate the evaporation rates and work out relative humidity from there. Wolfe's method was limited by the fact that ^{18}O levels are a function of temperature of formation and fluid composition in the time between sample formation and sample recovery - clumped isotope thermometry enables constraints on temperature, allowing improved estimation of actual ^{18}O levels at sample formation times and thus much better values for relative humidity.

  This was a welcome development as it would have enabled us to determine millenia-long changes in relative humidity over the Tropics, providing a tighter fit to our model as well as providing valuable data for other paleoclimatic approaches.

I presented a well received preliminary poster in September 2014 at UCLA's Science Poster Day, an open event showcasing undergraduate research, in line with the program's goal of facilitating scientific communication skills.

Challenges

A number of challenges were encountered in the development of this work:

- On the experimental front, a first run of the samples through our experimental apparatus indicated strong evidence of contamination from unknown sources. The source of this contamination was not identified - an early hypothesis, that nitrocellulose filter paper particles used in sample cleaning may have contaminated the particles, was discounted when it was discovered that nitrocellulose fiber is not converted to carbon dioxide on reaction with orthophosphoric acid, implying that the fiber was never actually fed into the spectrometer and alter our measurements. Procedures to prevent contamination, obtained in writing, had been followed meticulously at the time.

  We attempted to resolve this issue by redoing sample cleaning, on the off chance that an important step had been overlooked. Owing to the limited amount of sample available to us - sample weights ranged between 100 to 500 mg at best - it was agreed that the cleaning process would be done instead by experienced graduate students within Dr. Tripati's lab, a policy later extended to all incoming samples in the lab. A backlog of other samples with greater priority, however, delayed sample cleaning for several months, upto and including the last few months of this internship. We were thus never able to actually obtain temperature and δ^{18}O levels from sample data.

- Trial runs of our initial model on test data predicted a runaway warming effect with unrealistic time frames. By way of example, a temperature of 28°C was predicted to have become 500° C in a 'short' time span of 500 years - well past the boiling point of water. Ideally, we were looking for a model that could reasonably reproduce changes in sea surface temperature over the last century (approximately 1 degree Celsius or so). It became clear that the first iteration of our model did not meet this criterion.

  On Dr. Susan Hoban's advice, the stipulation of eighteen different interacting layers was removed and replaced with exactly one intervening layer, and model results compared with equilibrium values from other similar one-layer models. These models all converge to a specific value of about 255 K - a value that my model could not reproduce. This realisation prompted the view that the model itself was physically flawed and could not be fixed by ad-hoc amendments or additional information. In particular, using specific heat as a determinant of temperature increase was determined to be the root cause of model failure: specific heat necessitates the use of energy units, making the computation time dependent but also incorporating effects over the entire Earth. A better model, it seemed, was needed.

  The alternative approach I considered was to extend the mechanisms in these single-layer models to a multi-layer model. These models segment outgoing radiation from incoming radiation into reflected, transmitted and absorbed radiation in the atmosphere and the Earth, and assume energy conservation to calculate a final equilibrium temperature for all layers in the atmosphere. For a single layer, this is a

[3] *Reconstruction of paleohydrology and paleohumidity from oxygen isotope records in the Bolivian Andes*, Brent B. Wolfe, Ramon Aravena *et al.*, *Palaeogeography, Palaeoclimatology, Palaeoecology* 176 (2001) 177-192

set of linear equations; for two layers, this becomes a set of two coupled equations, and so on - the rank R of the resulting matrix equation increases linearly with the number of layers N. This is a 'textbook' one-dimensional model.

- Implementing the alternative approach ran into a number of difficulties, mostly conceptual. The chief issue was that descriptions of such a multi-layer model in the literature appear to inconsistently discard influences from other layers. For instance, reflected radiation off of the top of the lower layer in a two-layer model would not be included in the energy balance at the bottom of the upper layer. An attempt to independently derive the conclusions of this toy model by incorporating such interaction could not reproduce this result.

  We attempted to resolve this issue by contacting a colleague of Dr. Tripati's, Aiden Jönsson, a graduate student in atmospheric physics. Aiden Jönsson kindly provided us code that he had written in the past for multilayer modelling - it simulated the behaviour of ten to thirteen layers in MATLAB, but assumed certain fixed and different values of optical thickness for each layer, from which model parameters were calculated. Accounting for the impact of relative humidity on optical thickness proved to be a challenging task that was ultimately never resolved; to our knowledge, no work has ever been done in this regard, and a first principles approach invoking molecular composition and absorption spectra was beyond our capabilities. We ended up with a working model that we could not realistically refactor for our purposes.

Conclusion

Challenges to the project began to outweigh the progress partway through, and, at the time of writing this final report, a large number of technical and conceptual challenges still remain before objectives can be said to have been met. In retrospect, this project may simply have been too ambitious to undertake - it required combining several interdisciplinary theoretical and experimental approaches in a two-year time span, leaving little margin for errors that, possibly owing to inexperience on my part, cropped up. Research, it seems, does not follow a timeline.

Acknowledgements

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Appendix

Future Plans

My future plans, at the time of writing, have not been fixed.

Originally, I planned on enrolling into a doctoral program in physics. However, my experience with research and my interaction with other doctoral students has made me realise that I still have a long way to go before I am ready to be a doctoral candidate. More than anything else, my experiences have taught me the impact that errors on my part have on other people, and that approaching how to analyse and prevent errors and flaws in a setup is still something I need to work on. My strengths and weaknesses, I feel, do not yet overlap with the skills needed to perform high-calibre research. I have since decided to postpone my plans for involvement in research at the doctoral level, at least until such time as I feel I am actually able to handle the responsibility that comes with an independent research project.

For the time being, then, my focus has shifted towards developing myself professionally. I was not satisfied with the end result of my internship, and I feel that I should do what is in my power to prevent a similar occurrence happening again with future projects. The NASA PDS program did make me realise that I genuinely enjoyed designing programs, and I chose to join, as a consequence, a more computationally-oriented lab under Dr. Yuri Shprits, who leads the Space Environment Modelling group that studies extra-planetary plasmas. At the time of writing, I have begun to move incrementally towards the idea of writing high-performance code full-time, and thus towards becoming a software engineer.

From a professional perspective, this may constitute a drastic change in plans - from a personal perspective, however, I feel that experience working in such an environment will enable me to improve upon my weaknesses. The expectations of academia and industry are quite different, and I am confident that I will be able to improve myself in the other world. I am interning at DataWeave, a big data analytics startup, for the summer of 2015. I may pursue a Masters in Computer Science later on, or seek a full-time job, following this experience.